Multiscale Characterization of bcc Crystals Deformed to Large Extents of Strain

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Experimental data are crucial in the process of constructing and validating the multiscale crystal plasticity models used in computer code simulations of materials deformed under extreme conditions, such as high strain rate, high pressure, and large extents of strain. The "6 Degrees of Freedom" (6DOF) experiment was designed specifically for this task and has provided data on the behavior of bcc crystals that may revolutionize the field.

Until now, the experimental data and simulation efforts have focused on relatively small extents of plastic deformation (0.5%). Both experiments and modeling must now be extended to large strain deformations on the order of tens of percent. At these larger extents of strain, the use of multiscale characterization tools can be improved to better understand the fundamental behavior.

Project Goals

The goal of this project is to develop large strain experiments that will provide the essential data to enhance the multiscale modeling capability through the validation of dislocation dynamics simulations and the development of continuum strength models. This work will increase LLNL's ability to develop predictive strength models for use in computer code simulations.

Relevance to LLNL Mission

Understanding and simulating the plastic, or non-reversible, deformation of body-centered cubic (bcc) metals, is a major component of LLNL's stockpile stewardship mission, and is applicable to future NIF experiments.

FY2006 Accomplishments and Results

Slip System Analysis. Previous years' accomplishments included incorporating a full-field 3-D image correlation strain measurement system into the 6DOF experiment. Sequential photos are compared to determine the local movement of spots. Unlike traditional testing techniques, the 6DOF experiment allows essentially unconstrained deformation of the crystal. This unique set-up, shown in Fig. 1, allows for an unprecedented examination of the deformation of single crystals, including the complete displacement gradient matrix. Using this technique, we have performed an analysis that calculates the activity of individual slip systems in a single crystal from the image correlation data. The results for zinc single crystals are that for a pristine sample only the primary system is active, as expected. However, for a cold-worked and annealed sample, the analysis shows the unexpected result that there is appreciable activity on the primary as well as other slip systems.

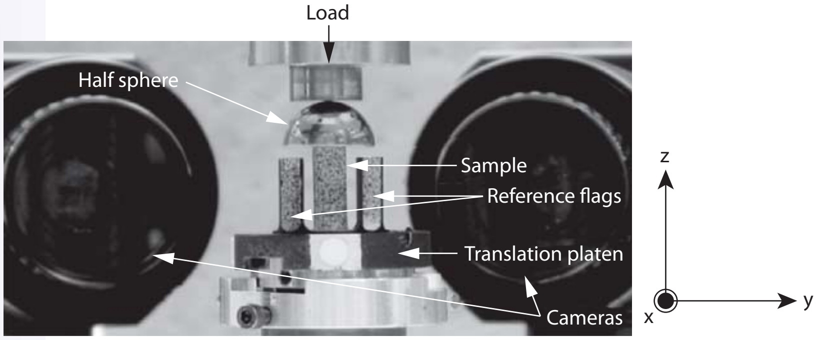

Figure 1. 6DOF set-up with the image correlations cameras.

Copper single crystals experiments. Experiments have been performed on copper single crystals that have also shown surprising results. The image correlation strain map (Fig. 2) shows slip along the primary (expected) and orthogonal to the primary slip system (unexpected). Using the image correlation data, analyses have been conducted that show that the slip is orthogonal and in some cases nearly equal in magnitude to the primary system. Additional experiments addressing the effect of fabrication and boundary conditions on the deformation behavior also show appreciable deformation orthogonal to the primary system. This behavior cannot be explained using traditional theories. In addition, orthogonal slip has been observed in hcp and bcc crystals, and therefore may be a general mechanism that can be applied to a large number of materials.

Characterization of the deformed material. Characterization of the deformed material, which is more definitive at larger strains, is essential to understanding the underlying deformation mechanisms in single crystal metals. One method of characterizing the deformed material is using the x-ray microdiffraction beamline at the Advanced Light Source (ALS) at LBL. The high-energy synchrotron light source allows subsurface dislocation structure to be analyzed. This technique can detect features over a larger area than is possible with Transmission Electron Microscopy (TEM). Copper single crystals, which show the orthogonal slip, have been characterized at ALS using x-ray microdiffraction. Figure 3, which is a map of the local rotations in the sample, shows band structures in the material that are 90º from each other. This result suggests that the local lattice rotations are related to the overall orthogonal structure seen in the image correlation strain maps.

Related References

1. Lassila, D. H., M. M. LeBlanc, and G. J. Kay, "Uniaxial Stress Deformation Experiments for Validation of 3-D Dislocation Dynamics Simulations," *J. Eng. Mat. Tech.*, **124**, p. 290, 2002.
2. LeBlanc, M. M., J. N. Florando, D. H. Lassila, T. Schmidt, and J. Tyson, II, "Image Correlation Applied to Single Crystal Plasticity Experiments and Comparison to Strain Gage Data," *Experimental Techniques*, **30**, 4, p. 33, 2006.

FY2007 Proposed Work

Further experiments and characterizations are needed to solidify the observation of orthogonal slip. Also, new theories and models, such as a dislocation dynamics simulation that takes into account local lattice rotations, need to be developed to account for this behavior.

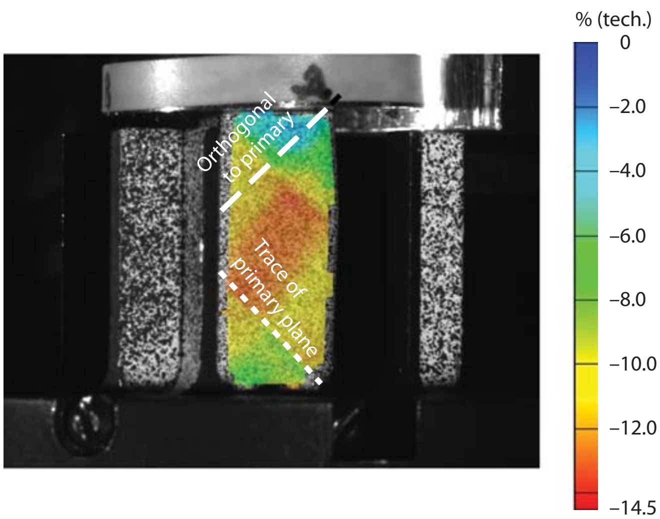

Figure 2. Axial strain map of copper single crystal overlaid onto the sample, showing deformation on the primary slip system and orthogonal to the primary system.

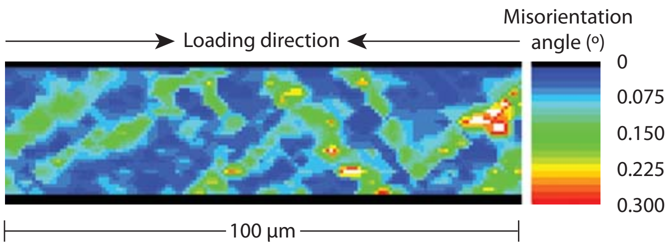

Figure 3. ALS results showing bands that are 90º from each other.